International Journal of Modern Physics E

PARTICLE NUMBER CONSERVING APPROACH TO CORRELATIONS

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Received October 19, 2006

In the present work the so-called Higher Tamm-Dancoff Apporximation method is presented for the generalized case of isovector and isoscalar residual interactions treated simultaneously. The role of different particle-hole excitations and of proton-neutron pairing correlations in the ground state of the self-conjugate ^{64}Ge nucleus is discussed.

PACS: 21.10.Hw, 21.60.Jz, 21.60.Cs

1. Introduction

It was recognized already in the sixties that the proton-neutron pairing may play a non-negligible role in the nuclei with equal numbers of protons and neutrons due to the particulary large spatial overlaps of the wave functions of both types of nucleons. One of the first methods developed to take into account such correlations were BCS-type approaches.[1,2,3,4,5,6] It is however known that the BCS wave function violates the particle number conservation which is especially harmful in the cases of weak pairing and phase transitions. A generic feature of the results of BCS calculations generalized so as to accomodate neutron-proton correlations (*i.e.* that take into account isoscalar and isovector pairs) in self-conjugate nuclei is a sharp transition from like-particle to $T = 0$ pairing modes. Such a scenario is absent in the particle number conserving approaches which allow for the coexistence of different superfluid phases.[7,8,9]

In the present study we propose an approach which is free of the deficiencies of the treatments à la Bogoliubov. This method, called Higher Tamm-Dancoff Approximation (HTDA), was already applied to study ground and isomeric states in heavier nuclei and to describe pairing correlations in high spin states.[10,11] Here we extend the HTDA formalism to take into account the proton-neutron pairing.

2. The HTDA framework

The purpose of the method is to describe the pair diffusion phenomenon around the Fermi surface as a particular, yet very important, part of some many quasiparticle excitations of the particle-hole type over a Slater determinant vacuum $|\Psi_0\rangle$. Thus one can consider dealing with a kind of higher Tamm-Dancoff approximation or equivalently with a highly truncated shell-model calculation. The latter point of view makes it clear that the success (*i.e.,* the fast convergence in terms of the number of considered quasiparticles) of such a truncation scheme will depend on the realistic character of the vacuum in use. Such a favorable situation may be expected when the vacuum is defined self-consistently from the mean-field carrying most of the single-particle (sp) properties (even those yielded by the correlations) associated with a given effective Hamiltonian

$$\hat{H} = \hat{K} + \hat{V}\,, \tag{1}$$

where $\hat{K}$ is the kinetic energy and $\hat{V}$ an effective interaction. It is advisable to choose for the wave function $|\Psi_0\rangle$ the Hartree-Fock solution coming from the HF potential $\hat{V}_{\rm HF}$ self-consistently obtained from the many-body reduced density matrix $\hat{\rho}$ of the correlated solution for the desired number of particles and possibly taking into account various constraints (*e.g.*, deformation) and symmetries (*e.g.*, time-reversal symmetry). We have thus

$$\hat{H}_{\rm HF}|\Psi_0\rangle = E_0|\Psi_0\rangle\,, \tag{2}$$

where

$$\hat{H}_{\rm HF} = \hat{K} + \hat{V}_{\rm HF}\,, \tag{3}$$

$\hat{V}_{\rm HF}$ being the one-body reduction of $\hat{V}$ for $|\Psi_0\rangle$.

The $|\Psi_0\rangle$ vacuum may now serve to construct an orthonormal N-body basis in which we will diagonalize Hamiltonian (1). In principle to build this basis we should consider the Slater determinant corresponding to the 0p0h state and all the particle-hole excitations: 1p1h $|\Psi_1\rangle$, 2p2h $|\Psi_2\rangle$, 3p3h $|\Psi_3\rangle$ and so on. It is however obvious that in practice we need to truncate the space of particle-hole excitations. Based on the former studies in the HTDA framework[10] we may assume that the components of the pair excitation type will be dominant in the ground state. In the section 3 we will show for the case of *pp* and *nn* correlations that the other components are indeed of a minor importance.

The total ground state wave function can be decomposed in the following way (τ and τ' denoting two different charge states)

$$\begin{aligned}|\Psi\rangle \equiv |\Psi^{\tau}\otimes\Psi^{\tau'}\rangle = \chi_{00}|\Psi_0^{\tau}\otimes\Psi_0^{\tau'}\rangle + \sum_{(\mathrm{1p1h})_{\tau}}\chi_{10}|\Psi_1^{\tau}\otimes\Psi_0^{\tau'}\rangle + \sum_{(\mathrm{1p1h})_{\tau'}}\chi_{01}|\Psi_0^{\tau}\otimes\Psi_1^{\tau'}\rangle \\ + \sum_{(\mathrm{1p1h})_{\tau}(\mathrm{1p1h})_{\tau'}}\chi_{11}|\Psi_1^{\tau}\otimes\Psi_1^{\tau'}\rangle + \sum_{(\mathrm{2p2h})_{\tau}}\chi_{20}|\Psi_2^{\tau}\otimes\Psi_0^{\tau'}\rangle + \sum_{(\mathrm{2p2h})_{\tau'}}\chi_{02}|\Psi_0^{\tau}\otimes\Psi_2^{\tau'}\rangle \\ + \cdots\end{aligned} \tag{4}$$

The ensemble of products of Slater determinants $|\Psi_i^\tau \otimes \Psi_j^{\tau'}\rangle$ represents a complete orthogonal basis of the N neutrons and Z protons physical space with real coefficients χ_m fulfilling the relation

$$\sum_m \chi_m^2 = 1 \tag{5}$$

which guarantees the normalization of the function (4). It is clear that this function has a good particle number $\langle\Psi|\hat{N}|\Psi\rangle = A$. To obtain the correlated ground state one should perform the diagonalization of the Hamiltonian (1) in the given many-body basis.

Let us rewrite the Hamiltonian (1) in the following form

$$\begin{aligned}\hat{H} &= \hat{K} + \hat{V}_{\rm HF} - \langle\Psi_0|\hat{V}|\Psi_0\rangle + \hat{V} - \hat{V}_{\rm HF} + \langle\Psi_0|\hat{V}|\Psi_0\rangle \\ &= \langle\Psi_0|\hat{H}|\Psi_0\rangle + \hat{H}_{\rm IQP} + \hat{V}_{\rm res}\,,\end{aligned} \tag{6}$$

where the independent quasiparticle Hamiltonian $\hat{H}_{\rm IQP}$ reads

$$\hat{H}_{\rm IQP} = \sum_i \xi_i \eta_i^\dagger \eta_i\,, \tag{7}$$

where $\eta_i^\dagger$ is the particle creation operator $a_i^\dagger$ for i being a particle (unoccupied) state and to the anihhilation operator a_i in the case of hole (occupied) states. For ξ_i we have: $\xi_i = e^i$ or $\xi_i = -e^i$, with e^i indicating the single-particle (HF) energy corresponding to the particle or hole case, respectively. As seen from Eq. (6), the residual interaction reads

$$\hat{V}_{\rm res} = \hat{V} - \hat{V}_{\rm HF} + \langle\Psi_0|\hat{V}|\Psi_0\rangle\,. \tag{8}$$

The matrix element of the above given Hamiltonian in the multi-particle multi-hole basis takes the form

$$H_{ij} = \left(\langle\Psi_0|\hat{H}|\Psi_0\rangle + \sum_{\tau=p,n} E_{\rm p-h}^{i\tau}\right)\delta_{ij} + \langle\Psi_i|\hat{V}_{\rm res}|\Psi_j\rangle\,, \tag{9}$$

where $\sum_{\tau=p,n} E_{\rm p-h}^{i\tau}$ is the total particle-hole excitation energy calculated with respect to the vacuum $|\Psi_0\rangle \equiv |\Psi_0^\tau \otimes \Psi_0^{\tau'}\rangle$. The residual interaction comprising only one- and two-body operators will merely contribute to the matrix elements in cases where the two many-body states are identical or differ by one or two particles. The many-body matrix elements of $\hat{V}_{\rm res}$ can be evaluated with the use of the Wick theorem (for details see Ref.[12]) and expressed as sums of proper two-body matrix elements of the interaction $\hat{V}$.

In actual calculations with our approach we have used the Skyrme force for the HF part of the problem. Since the majority of the Skyrme forces is not well suited to reproduce the data in the particle-particle channel we apply a δ-force to define the residual interaction. Using the zero-range force is well established in the context of like-particle and– to a lesser extent– of the proton-neutron pairing. To

assess the validity of our approach at this early stage of the investigation of the proton-neutron correlations within the HTDA framework a substitution

$$\hat{V} \Rightarrow \hat{V}_\delta = \sum_{T=0,1} V_0(T)\delta(\vec{r}_{12})\Pi^S\Pi^T \tag{10}$$

is therefore done for the residual interaction. The operators $\Pi^S\Pi^T$ project onto spin-isospin subspaces

$$\hat{\Pi}^S = \frac{1}{2}(1-(-1)^S P^\sigma)\,, \tag{11}$$

$$\hat{\Pi}^T = \frac{1}{2}(1-(-1)^T P^\tau)\,, \tag{12}$$

where $P^\sigma = 1/2(1-\vec{\sigma}_1\cdot\vec{\sigma}_2)$, $P^\tau = 1/2(1-\vec{\tau}_1\cdot\vec{\tau}_2)$ are the standard spin and isospin exchange operators.

3. Results

The main challenge in the exact pairing diagonalizations methods and shell-model like calculations is the large dimension of the matrix to be diagonalized. In the present study we use the Lanczös algorithm[13] within the code developed by Parlett and Scott[14] which allows to search for the lowest energy solutions in a reasonable time. However, as will be shown in the following, the advantage of the HTDA method is that the amount of the many-body configurations within a given single-particle space that need to be taken into account is quite limited and the matrix diagonalization problem is far from attaining the difficulty level of typical shell-model calculations.

The calculations within the HTDA framework which we will discuss here are performed for the ground state of the ^{64}Ge nucleus as obtained in a Skyrme-HF+BCS approach. We use the SIII force for the particle-hole channel, seniority force in the BCS part and volume δ interaction to calculate two-body matrix elements in the HTDA part. The HTDA results presented here are non self-consistent. Indeed, only one diagonalization of the HTDA Hamiltonian matrix has been carried out for a Hamiltonian $\hat{H}_{\rm HF}$ obtained with the density $\hat{\rho}$ corresponding to the HF+BCS calculation.

3.1. *Limiting case: pp and nn interactions*

In the limiting case of vanishing proton-neutron correlations we obtain two decoupled problems, one for each charge state. Let us discuss first the aspects of the basis truncation, both in single-particle and many-particle many-hole excitations terms. If the assumptions of the BCS theory are to hold, we may expect that the most important part of the ground state correlations will correspond to the pair excitations, *i.e.* the situation where two particles in Kramers degenerate hole orbitals are promoted to two Kramers degenerate particle levels. In what follows we will restrict the many-body states first to take into account all possible 1p1h and 2p2h

Table 1. Numbers of many-body configurations of different types depending on the number of sp levels in the window.

Number of sp levels	1p1h	1 pair	2p2h	2pairs	3 pairs
12	10	40	260	280	560
20	22	96	1744	1848	12157
28	48	180	6596	6758	58404
36	76	260	13706	14230	>100000

excitations including thus the one pair excitations in addition to the particle-hole vacuum. In further calculations only the states corresponding to one, two and three pairs excitations will be considered.

Having chosen a configuration space size in terms of the complexity of many-particle many-hole states, one has to further truncate on single-particle levels from which these configurations will be built. We are facing thus a situation met in customary BCS calculations. Typically, we will limit our sp subspace to the so-called configuration space window defined as

$$e_F \pm E^{\rm sp}_{\rm cut}\,, \tag{13}$$

where e_F is the Fermi energy (defined as the average between the single-particle energies of the last occupied and first unoccupied levels) and $E^{\rm sp}_{\rm cut}$ the cut-off energy. The actual value of the latter should be chosen such that the inclusion of additional sp levels does not introduce any significant physical consequences but only a possible slight renormalization of the relevant quantities. In Table 1, to exemplify the matrix dimensions, we give numbers of configurations corresponding to different particle-hole excitations depending on the number of sp levels included in the configuration space window.

Since in the HTDA calculations we are using a δ-force it is clear that both the coupling constant and the cut-off parameter are necessary to define fully the interaction. It is then indispensable to fix the δ-force strength in our approach to reproduce physical quantities, *e.g.*, the phenomenological 3-point gaps for the considered nucleus (Δ_n=1.48 MeV, Δ_p=1.14 MeV evaluated with experimental masses of Ref.[15]). Assuming that the appearance of the pairing gap is related to a breaking of the Cooper pair of the lowest energy, we perform the HTDA calculations with one level (neutron or proton) closest to the Fermi energy blocked and adopt the difference of the expectation value of $\hat{V}_{\rm res}$ in the two calculations as a proper measure of the pairing correlations that can be compared to the experimental odd-even mass differences. Namely, we define

$$\Delta = [E(n) - E_{\rm IQP}(n)] - [E(n-1) - E_{\rm IQP}(n-1)]\,, \tag{14}$$

Table 2. Percentage of different components of the ground state correlated wave function. The results concern the case where all types of particle-hole excitations up to the 2nd order are taken into account.

	0p0h	1p1h	1 pair	2p2h (all included)
neutrons	69.6	0.003	29.6	30.4
protons	70.6	0.005	29.3	28.3

where $E = \langle\Psi|\hat{H}|\Psi\rangle$, $E_{\rm IQP} = \langle\Psi|\hat{H}_{\rm IQP}|\Psi\rangle$ and n indicates the number of sp levels in the configuartion space window. Since we deal with the $N = Z$ nucleus one value of the coupling constant V_0 and of the cut-off energy $E^{sp}_{\rm cut} = 10$MeV is adopted for both charge states in further calculations.

First, let us discuss the result of the diagonalization of the Hamiltonian matrix in the many body basis containing all 1p1h and 2p2h components. The decomposition of the correlated function for neutrons and protons is given in Table 2. As expected, the main contribution beyond the 0p0h vacuum comes from one pair excitations. The 1p1h part is fully negligible while the 2p2h excitations of other types constitute less than 1% of the correlated wave function so restricting the many-particle many-hole excitations to study only pair excitations in addition to the vacuum seems well justified. Of course it allows for a great simplification from the calculational point of view, as the number of pair excitations is very modest as compared to the number of all possible particle-hole excitations (cf. Tab. 1).

The same procedure is employed in the case of calculations where one, two and three pairs excitations in addition to the vacuum are considered. In Table 3 the decomposition of the correlated wave function is given for neutrons and protons in three cases: when only 1 pair excitations are considered in addition to the vacuum state, when 2 pairs are added and finally, when 3 pairs are as well embedded in the calculations. We also give the corresponding values of the correlation energy defined as the difference of the mean values of the Hamilton operator of the system in correlated and uncorrelated states

$$E_{\rm corr} = \langle\Psi|\hat{H}|\Psi\rangle - \langle\Psi_0|\hat{H}|\Psi_0\rangle\,. \tag{15}$$

As seen, one pair excitations contribute the most in all cases, two pairs excitations give only about 2% of the total amount while the probability for three pairs is negligible. Including the latter has a minimal influence on both the correlation energy and on the percentage of other components. However, the presence of two pairs boosts the population of the one pair excitation content of the correlated wave function, as already observed in the calculations of Ref.[12]. This entails that to describe accurately the one pair excitation phenomenon two pair transfers are a priori needed. Nevertheless, at this early stage of our study of proton-neutron pair-

Table 3. Percentage of various components of the correlated wave function and the correlation energy values for neutrons and protons. Results of three calculations are reported: with 1 pair excitations added to the vacuum, with 1 and 2 pairs and with 1, 2 and 3 pairs included.

	0p0h	1 pair	2 pairs	3 pairs	$E_{\rm corr}$ (MeV)
neutrons	65.4	34.6	–	–	-1.16
	49.55	48.5	1.95	–	-1.43
	49.0	48.9	2.1	0.02	-1.45
protons	65.3	34.7	–	–	-1.18
	47.7	50.2	2.1	–	-1.48
	46.9	50.7	2.3	0.04	-1.50

ing correlations we will exclude 2 pairs components for obvious practical reasons.

3.2. *General case: $T = 1$ and $T = 0$ pairing interaction*

As we already stated we aim at including the $T_z = 0$ pairing correlations within the HTDA framework. As above discussed in this preliminary study we limit the configuration space to the so-called one pair excitations in all channels.

Since proton-neutron pairs may exist in both $T = 0$ and $T = 1$ channels the problem of adjusting the strength of the isoscalar pairing arises here. The interplay of $T = 0$ and $T = 1$ pairing being rather unclear, we will adopt the same value of the isovector pairing strength for *pp*, *nn* and *pn* channels and will treat the $T = 0$ interaction strength as a free parameter.[a]

Within a given configuration space and $T = 1$ strength adjusted as described in the precedent we perform the calculations as a function of the increasing $T = 0$ coupling constant. In Fig. 1 the evolution of the probability of different components is plotted against the ratio

$$x = V_0(T = 0)/V_0(T = 1)\,. \tag{16}$$

The probability of the $T_z = 0$ pair excitation becomes siginificant with respect to that of *pp* or *nn* pair excitation for $x > 2$ which corresponds to the ratio value at which a *pn* superfluid solution is found in BCS(δ)-type of calculations in this nucleus.[9] The gain in energy due to the *pn* coupling is non-negligible which can be

[a]A considerable amount of *pn* pairing correlations can be as well obtained in an isospin broken model with $V_0^{\tau\tau'} > V_0^{\tau\tau}$, nevertheless we do not see any argument supporting such a choice.

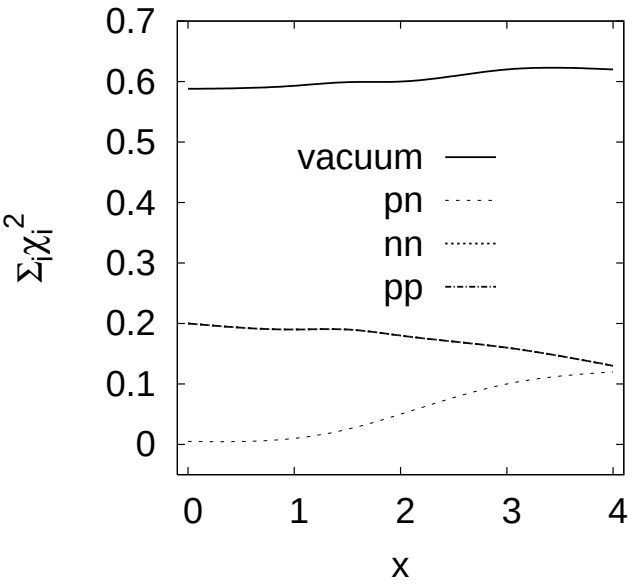

Fig. 1. Total probability of different type of components (vacuum-$(0p0h)_p \otimes (0p0h)_n$, pn-$(1p1h)_p \otimes (1p1h)_n$, pp-$(0p0h)_n \otimes (2p2h)_p$, nn-$(2p2h)_n \otimes (0p0h)_n$) in the correlated wave function $|\Psi\rangle$ versus the ratio x of the δ-force strengths in isoscalar ($T = 0$) and isovector ($T = 1$) channels.

seen from Fig. 2 where the contribution of different components to the correlation energy is depicted. It is worth noting that the increase of the energy is of a similar magnitude like that of BCS calculations with the approximate particle number projection of the Lipkin-Nogami (LN)[9] nonetheless a certain gain in the HTDA correlation energy due to the *pn* coupling occurs already in the range of parameters for which no *pn* pairing solution is found in the BCS+LN method ($x \leq 2$).

4. Summary

We have presented a method explicitely conserving particle number in the context of describing isovector and isoscalar pairing correlations. The inclusion of $T = 0$ pairs leads to a constant increase of the absolute value of the correlation energy. The expected benefit of the HTDA framework in yielding a much smoother decrease of correlations than when using a Bogoliubov quasiparticle vacuum in weak pairing regimes is confirmed.

5. Acknowledgements

One of the authors (K.S.) is indebted to Jacek Dobaczewski for fruitful discussions. This work is partly supported by the Committee of Scientific Research (KBN) of the Polish Ministry of Science and Education under contract No. 1P03B13028

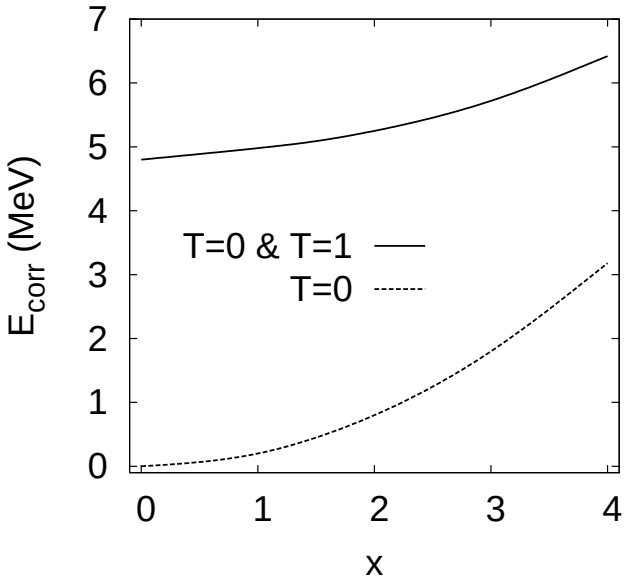

Fig. 2. Absolute value of the correlation energy plotted against the ratio x of the interaction strengths in isoscalar and isovector channels. The results concern calculations with $T = 0$ pn pairs only and with all possible pairs taken into account.

(2005-2006) and the French Embassy in Poland.

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